Lagrangian Modeling at Sandia National Laboratories: Current Status and Future Directions

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Efficient Lagrangian methodologies for quadrilaterals and hexahedral meshes have been available for a number of years. Mesh generation issues for complex three-dimensional geometries can, however, be a severe limiting factor. Mesh generation for triangular and tetrahedral meshes is readily available, but solid mechanics discretizations on these meshes are not so well established because of problems with locking. We review a relatively new node-based uniform strain element as well as an SUPG stabilized formulation that hold promise for effective simulations using a more general suite of elements.

Introduction

Lagrangian hydrodynamic and solid dynamic modeling represents a key modeling technology for Sandia National Laboratories. Applications for Lagrangian technology range from quasi-static and transient dynamic Lagrangian modeling to Lagrangian time stepping embedded in arbitrary Lagrangian Eulerian frameworks for high energy, shock physics applications. Commonly used transient dynamic and quasi-static modeling methodologies are based on updated Lagrangian formulations using a uniform strain element on quadrilateral and hexahedral meshes with a central-difference time discretization. For some applications structural elements are required and, in addition, contact algorithms must be implemented in a scalable way. Typically, stresses are updated using a mid-point increment formulation associated with a polar objective rate or with an incremental stress formulation. The basic Lagrangian methodology commonly used at Sandia is based on the PRONTO3D Lagrangian code (Taylor and Flanagan, 1987) with quadrilateral and hexahedral uniform strain elements. These elements require hourglass control and an explicit artificial viscosity treatment to deal with shocks. Parallel computation uses a spatial domain decomposition approach in which the element patches are created and subsequently loaded into appropriate processors on a distributed memory machine. Contact algorithms are an important part of the overall Lagrangian modeling capability (Brown, et al., 2003).

Unfortunately, the quadrilateral and hexahedral technologies can be problematic due to difficulties with mesh generation, ad hoc hourglass control, and the inability of the formulations to well represent gradients on arbitrary meshes. Triangular or tetrahedral elements present some advantage relative to "brick"-type elements, being amenable to

advanced automatic mesh generation, with a consistent reduction of the overall finite element analysis time. Typical implementations make use of a constant discontinuous approximation for the pressure, resulting in excessive element stiffness, which ultimately produces the so-called element "locking" in the incompressible limit. Thus these simplicial element types have been avoided in the past.

Newer numerical formulations may provide additional flexibility for Lagrangian modeling. This paper provides a brief overview of two such new technologies. We describe below a new nodal tetrahedral element that provides much improved properties over the classical tetrahedral element formulation while allowing for the use of more easily generated meshes. Subsequently, we describe a new SUPG stabilized formulation for Lagrangian hydrodynamics that provides an alternative framework for a nodal based, robust, topology-independent methodology.

A node-based uniform strain Lagrangian element

Sandia has a long history of searching for triangular and tetrahedral element technologies that will match the quality and efficiency of average gradient quadrilateral and hexahedral elements (Dohrmann, et al., 1998; Key, et al., 1999). The most promising approach is termed the node-based uniform strain element (Dohrmann, et al., 2000). This approach uses linear shape functions on triangular and tetrahedral elements to construct a gradient approximation centered at nodes. By extending the stencil and placing the stresses at the nodes, one obtains an optimal constraint ratio and elements that perform quite well at a slightly higher cost. This is seen as a reasonable tradeoff when rapid results are needed on new geometries and the cost of mesh generation must be taken into account. Figure 1 illustrates the stencil constructed around a node in the case of triangles. Each element of area, A_J , can be related to an average gradient operator via

$$B_{Jik} = \partial A_J / \partial x_{iJ_k} \tag{1}$$

$$A_J = x_{iJ_k} B_{Jik} \tag{2}$$

The B matrix gives the average gradient operator for element J. One then needs to develop gradient operators associated with the virtual hexagons surrounding each node in the figure. To this end one defines a partitioning

$$1 = \alpha_{J_1 J} + \alpha_{J_2 J} + \alpha_{J_3 J} \tag{3}$$

such that

$$\widehat{A}_L = \alpha_{LJ} A_J \tag{4}$$

which gives

$$\widehat{B}_{LiI} = \partial \widehat{A}_L / \partial x_{iI} \tag{5}$$

and the assembled force at node I is given by

$$f_{iI} = \sigma_{ij}^L \widehat{B}_{LjI} . \tag{6}$$

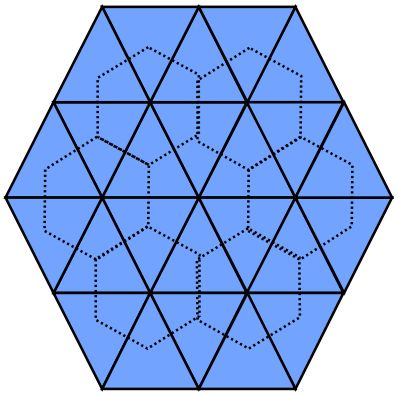

Figure 1: Stencil for node-based uniform strain element.

A common test of element performance is the Taylor bar impact problem (Johnson and Cook, 1983). In Figure 2 and Table 1 we compare an eight node hexahedral mesh with two tetrahedral formulations developed at Sandia, the eight node tetrahedron and the nodal based tetrahedron. Both tetrahedral formulations alleviate the well known locking phenomenon observed in the standard four node tetrahedral formulation. This example and others that have been investigated demonstrate that the nodal based tetrahedron has an equivalent performance in terms of cost/accuracy relative to the eight node hexahedron. In general, the nodal based tetrahedral mesh will have a smaller critical time step than the eight node hexahedral mesh. However, the increased CPU time associated with the smaller time step is offset by increased accuracy of the solution.

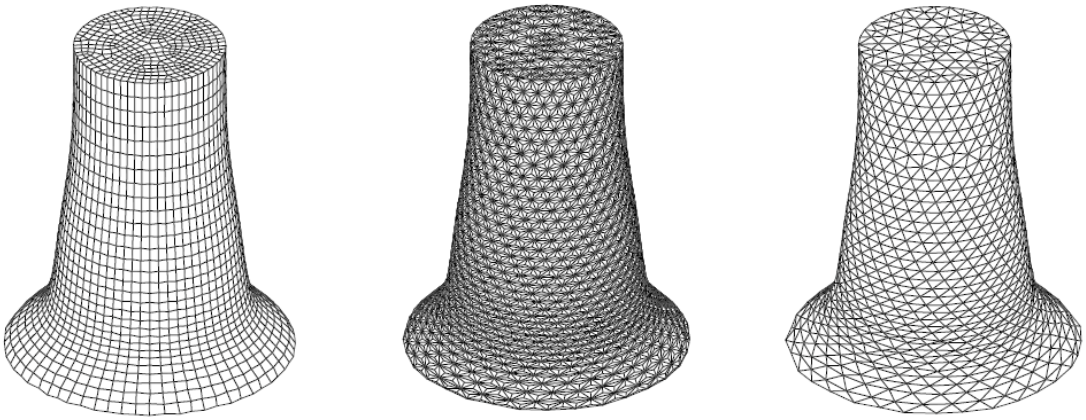

Figure 2: Taylor Bar impact comparison (Example courtesy of S.W. Key, J.D. Gruda and A.S. Gullerud.)

Table 1. Taylor bar impact comparison of numerical results with experiment. (Table courtesy of S.W. Key, J.D. Gruda, and A.S. Gullerud.)

Element	Final Length	Base Diameter	Diameter @ 0.2 L_0

Hex-8	17.3 (mm)	14.6 (mm)	9.6 (mm)
Tet-8	17.2 (mm)	14.4 (mm)	9.4 (mm)
Nodal Based Tet	17.3 (mm)	14.6 (mm)	9.5 (mm)
Johnson-Cook	17.2 (mm)	14.6 (mm)	n/a
Experiment	16.2 (mm)	13.5 (mm0	10.1 (mm)

An SUPG approach for Lagrangian hydrodynamics

We now discuss an alternative approach, based on the Streamline Upwind Petrov-Galerkin formulation (Brooks and Hughes, 1982), resulting in a multidimensional formulation for the Lagrangian equations of gas dynamics. Equal order linear interpolation is adopted for *all* variables (namely displacements, velocities and pressures in the current formulation), which are centered at the mesh nodes. The globally continuous, piecewise-linear representation of the pressure field avoids problematic issues related to the reconstruction of its gradients. This last aspect is beneficial for brick-type elements since improved accuracy is gained with respect to traditional hydrocode implementations. To introduce the method, let us refer to the formulation in the original paper. A straightforward Galerkin discretization of the advection-diffusion equation

$$c\frac{\partial \phi}{\partial x} - \kappa\frac{\partial^2 \phi}{\partial x^2} = 0, \qquad (7)$$

results in the unstable central difference approximation of the derivative $\partial\phi/\partial x$. The upwind discretization is recovered by means of an appropriate numerical viscosity:

$$c\frac{\partial \phi}{\partial x} \cong c\left(\frac{\phi_{n+1}-\phi_n}{\Delta x}\right) = c\left(\frac{\phi_{n+1}-\phi_{n-1}}{2\Delta x}\right) + \frac{c\Delta x}{2}\left(\frac{\phi_{n+1}-2\phi_n+\phi_{n-1}}{\Delta x^2}\right) \qquad (8)$$

The use of such numerical diffusion operator in a finite element discretization would result in stability at the price of consistency and ultimately accuracy, since the addition of a numerical viscosity operator of this sort destroys the residual structure of the variational equations. The idea of Brooks and Hughes was to incorporate upwind in finite elements, from a variationally consistent point of view, by *perturbing* the test function space as in the following Petrov-Galerkin formulation (strong Dirichlet boundary conditions are assumed):

$$0 = \int_0^L (-w_{,x}c\phi + w_{,x}\kappa\phi_{,x} - wf)\,dx + \sum_{n=1}^{N_{el}} \int_{x_{n-1}}^{x_n} p(c\phi_{,x} - \kappa\phi_{,xx} - f)\,dx, \qquad (9)$$

$p = \tau c w_{,x}$ is the test function perturbation, with $\tau = \Delta x/(2|c|)\left(coth\left(Pe_h\right) - 1/Pe_h\right)$ and $Pe_h = |c|\Delta x/2\kappa$. The numerical viscosity concept is embedded in the formulation as the two-element assembly of the following perturbative term shows:

$$\int_{x_{n-1}}^{x_n} pc\phi_{,x}dx = \int_{x_{n-1}}^{x_n} w_{,x}\tau c^2\phi_{,x}\,dx = \int_{x_{n-1}}^{x_n} w_{,x}\frac{|c|\Delta x}{2}\phi_{,x}\,dx \;\Leftrightarrow\; \frac{|c|\Delta x}{2}\left(\frac{\phi_{n+1}-2\phi_n+\phi_{n-1}}{\Delta x^2}\right) \qquad (10)$$

It is possible to prove that the SUPG method yields a *nodally exact* solution for the linear advection-diffusion equation in one dimension, and that in the multi-dimension case, although nodal exactness is lost, optimal convergence rates still hold. SUPG stabilized methods were successfully generalized to advective-diffusive systems of equations and compressible Euler and Navier-Stokes equations during the decade 1986-1995 (Shakib, et al., 1991). In this case SUPG stabilization is applied along characteristics. The Lagrangian hydrodynamics equations in conservative and quasi-linear form read:

$$\begin{aligned} &\dot{U}(Y^h) + F_i(Y^h)_{,i} + Z(Y^h) - f = 0 \\ &A_0\dot{Y}^h + A_i Y^h{}_{,i} + CY^h - f = R(Y^h) = 0 \\ &\mathcal{L}_{adv} = A_0\partial_t + A_i\partial_{X_i} \end{aligned} \tag{11}$$

where U is the vector of conserved variables, expressed in terms of the discretized variables Y^h, A_0 and A_i are the Jacobians of the time flux, U, and the spatial fluxes, F_i, respectively. The weak form of the equations integrated over a space-time slab of thickness $[t_n, t_{n+1}]$ reads:

$$B(W^h, Y^h) + SUPG(W^h, Y^h) + DC(W^h, Y^h) = F(W^h) \tag{12}$$

$$\begin{aligned} B(W^h, Y^h) = &\int_V W^h(X, t_{n+1}) \cdot U(Y^h(X, t_{n+1}))\, dV - \int_V W^h(X, t_n) \cdot U(Y^h(X, t_n))\, dV \\ &- \int_{Q_n} W^h_{,i} \cdot F_i(Y^h)\, dQ + \int_{Q_n} W^h \cdot Z(Y^h)\, dQ + \int_{P_n^G} W^h \cdot F_i(Y^h) N_i\, dP \end{aligned} \tag{13}$$

$$SUPG(W^h, Y^h) = \sum_{e=1}^{n_{el}} \int_{Q_n^e} \mathcal{L}_{adv} W^h \cdot \tau R(Y^h) dQ \tag{14}$$

$$F(W^h) = -\int_{P_n^H} W^h \cdot H\, dP + \int_{Q_n} W^h \cdot f\, dQ \tag{15}$$

where H is the Neumann flux and $DC(W^h, Y^h)$ is an artificial viscosity operator of the von Neumann-Richtmyer type with Noh heat flux correction. In the above the trial functions, Y^h, are assumed linear in time and the test functions, W^h, are assumed piecewise constant in time. An explicit predictor/multi-corrector strategy is adopted to solve the nonlinear system of equations presented.

Numerical Results

A few numerical tests for the Euler equation in Lagrangian coordinates are reported here. The first test presented is a variant of the classical Sod test. Reflective boundary conditions are imposed at the two ends of the one-dimensional shock-tube domain, causing the shock wave generated in center of the domain to reflect on the right boundary and interact with the contact discontinuity. This example tests the ability of the method to deliver good solutions at the interface of the contact, where elements of very different size are next to one another. As shown in Figure 3, a standard hydrocode implementation

with HEMP viscosity (Benson, 1992) delivers very poor results when compared with the new approach. A large spike in the pressure and velocity completely destroys the features on the right of the contact discontinuity.

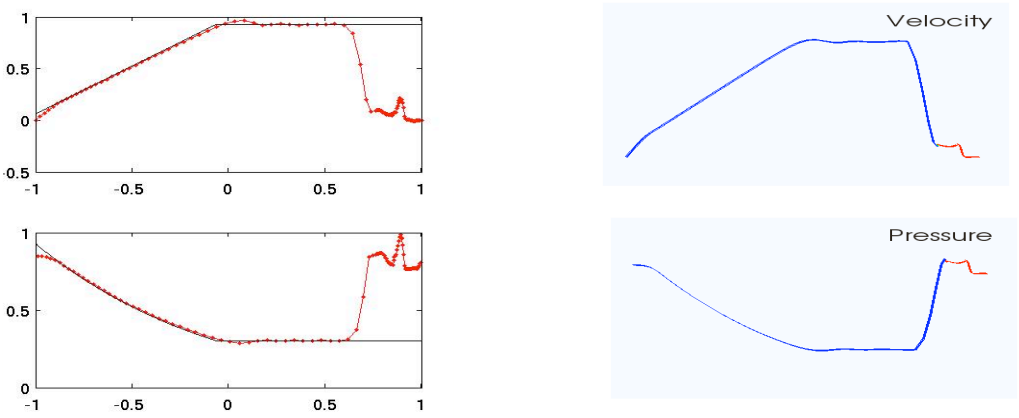

Figure 3. Sod test at T=0.9 (100-element mesh at CFL=0.9). Standard hydrocode (left) compared with the SUPG method (right). Top: velocity. Bottom: pressure. Notice the spurious spike present in the hydrocode solutions, absent for SUPG.

The second test (Figure 4) is the well-known Saltzmann piston test for a two-dimensional quadrilateral grid. The SUPG method ran long enough for the shock to reflect *six* times. We believe the test could have been run further, given the quality of the final solution.

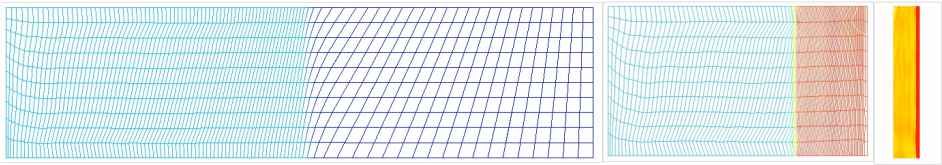

Figure 4. Saltzmann test, CFL=0.9. Snapshots of the pressure taken before the first shock reflection (left), after the first reflection (center), and after the fifth reflection (right). Notice the quality of the solution in terms of the alignment of the shock front and the alignment ofhorizontal mesh lines.

The third and last test presented is a Noh implosion test for a triangular mesh (Figure 5). Noticeable underheating is observed in the density profiles at the wall locations. Notice the absence of oscillations in the finite element solution.

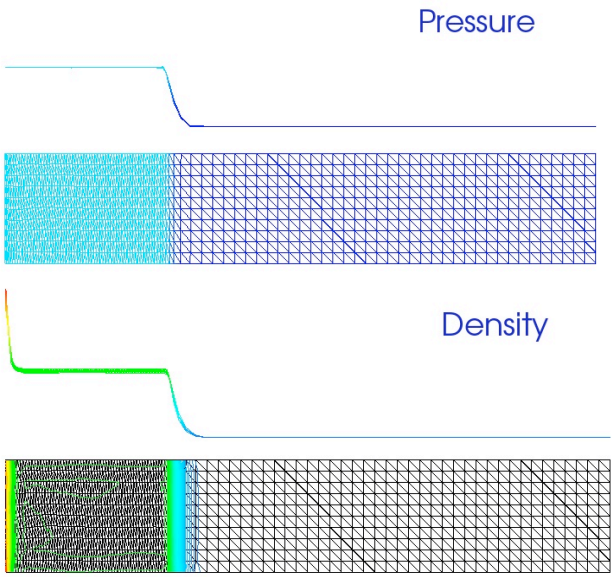

Figure 5. Noh test, triangular grid (aspect ratio 1:1), CFL=0.75, pressure (top) and density (bottom). Notice the smoothness of the density and pressure profiles.

Conclusions

Useful and efficient algorithms on simplicial meshes are being developed and compared favorably with older methodologies designed for quadrilateral and hexahedral meshes. These algorithms promise to lead to general techniques for solution of Lagrangian solid mechanics problems on more general finite element meshes.

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